



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:14 AM UTC

PDB ID : 2RGR / pdb_00002rgr
Title : Topoisomerase IIA bound to G-segment DNA
Authors : Dong, K.C.; Berger, J.M.
Deposited on : 2007-10-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

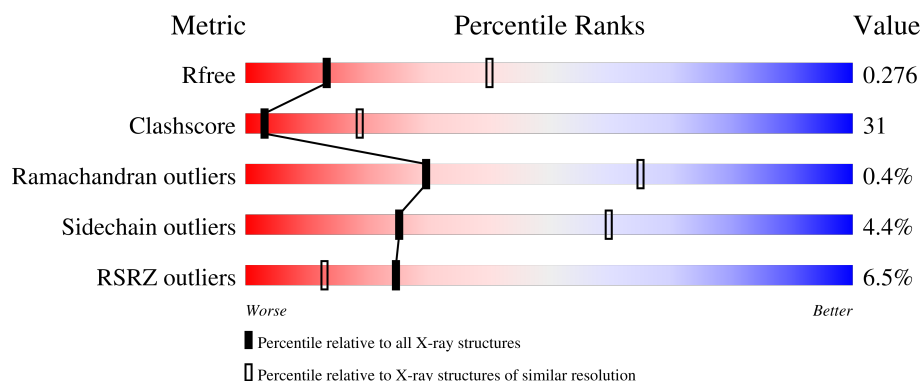
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	15	60% 40%
2	D	19	5% 21% 74% 5%
3	A	759	6% 52% 38% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	15	Total	C	N	O	P	0	0	0
			310	147	63	86	14			

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			380	181	67	114	18			

- Molecule 3 is a protein called DNA topoisomerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	721	Total	C	N	O	S	0	0	0
			5929	3823	995	1091	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	LEU	PRO	SEE REMARK 999	UNP P06786

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total	O	0	0
			6	6		

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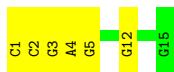
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	O	0	0
			3	3		
5	A	39	Total	O	0	0
			39	39		

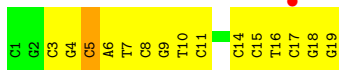
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

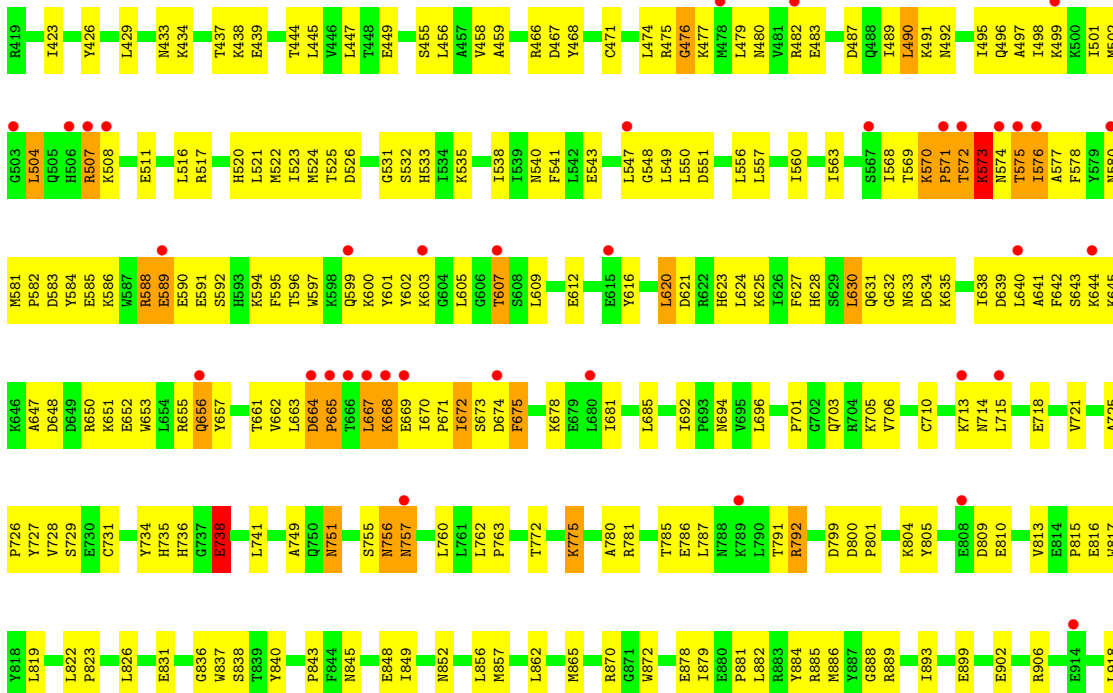
- Molecule 1: DNA

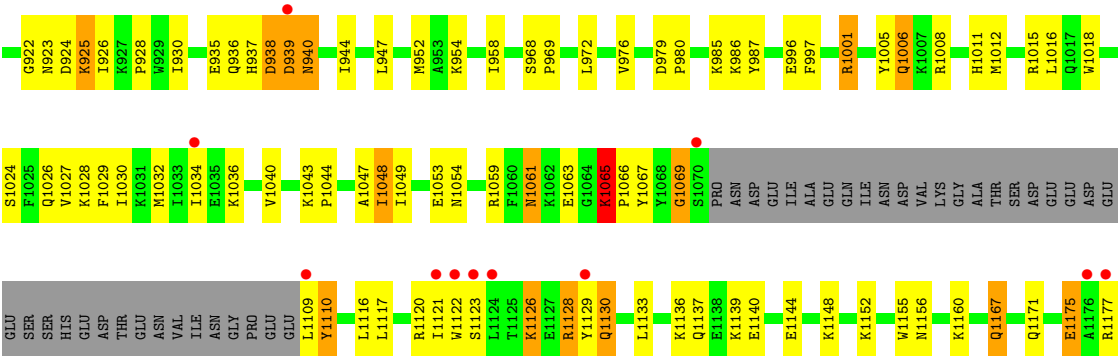


- Molecule 2: DNA



- Molecule 3: DNA topoisomerase 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 126.80Å 223.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 3.00 43.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.87-3.00) 99.6 (43.87-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.278 0.227 , 0.276	Depositor DCC
R_{free} test set	1255 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6668	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.32	0/349	0.97	0/538
2	D	0.36	0/423	1.12	5/649 (0.8%)
3	A	0.61	14/6066 (0.2%)	1.07	51/8179 (0.6%)
All	All	0.59	14/6838 (0.2%)	1.07	56/9366 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	576	ILE	CA-C	6.65	1.61	1.52
3	A	656	GLN	CD-OE1	5.54	1.34	1.23
3	A	940	ASN	CG-OD1	5.52	1.34	1.23
3	A	1006	GLN	CD-OE1	5.41	1.33	1.23
3	A	845	ASN	CG-OD1	5.37	1.33	1.23
3	A	1130	GLN	CD-OE1	5.27	1.33	1.23
3	A	756	ASN	CG-OD1	5.26	1.33	1.23
3	A	1054	ASN	CG-OD1	5.22	1.33	1.23
3	A	751	ASN	CG-ND2	-5.21	1.22	1.33
3	A	694	ASN	CG-OD1	5.11	1.33	1.23
3	A	845	ASN	CG-ND2	-5.08	1.22	1.33
3	A	1069	GLY	C-N	5.04	1.40	1.33
3	A	757	ASN	CG-ND2	-5.02	1.22	1.33
3	A	1061	ASN	CG-OD1	5.01	1.33	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	ARG	N-CA-C	15.75	134.43	109.39
3	A	938	ASP	N-CA-C	13.02	130.25	112.93
3	A	755	SER	N-CA-C	12.92	129.83	112.13
3	A	938	ASP	CB-CA-C	-11.42	92.16	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	939	ASP	N-CA-C	-10.49	88.46	110.80
3	A	621	ASP	N-CA-C	-9.47	100.50	112.90
3	A	665	PRO	CA-C-N	-9.00	109.53	123.13
3	A	665	PRO	C-N-CA	-9.00	109.53	123.13
3	A	1065	LYS	CA-C-N	8.82	128.76	120.03
3	A	1065	LYS	C-N-CA	8.82	128.76	120.03
3	A	573	LYS	N-CA-C	8.80	125.83	112.54
3	A	571	PRO	CA-N-CD	-8.51	99.58	111.50
3	A	547	LEU	N-CA-C	8.34	121.19	111.02
3	A	570	LYS	C-N-CD	8.07	138.36	120.60
3	A	675	PHE	N-CA-C	-7.94	102.22	111.03
3	A	755	SER	CB-CA-C	-7.48	99.01	110.83
3	A	756	ASN	N-CA-CB	7.48	122.52	110.77
3	A	939	ASP	N-CA-CB	7.46	123.11	110.49
3	A	664	ASP	O-C-N	7.39	128.91	121.30
3	A	507	ARG	CB-CA-C	-7.31	100.23	112.00
2	D	5	DC	N1-C1'-C2'	-7.12	102.83	113.50
3	A	925	LYS	N-CA-C	-6.90	106.76	114.62
3	A	642	PHE	N-CA-C	6.82	121.60	113.28
3	A	756	ASN	N-CA-C	-6.72	97.31	108.34
3	A	573	LYS	CA-C-N	-6.68	111.36	121.31
3	A	573	LYS	C-N-CA	-6.68	111.36	121.31
3	A	1036	LYS	N-CA-C	6.41	119.94	111.28
3	A	670	ILE	N-CA-C	-6.23	95.42	108.88
3	A	669	GLU	N-CA-C	-6.23	98.47	109.06
3	A	692	ILE	CA-C-N	5.97	126.43	120.52
3	A	692	ILE	C-N-CA	5.97	126.43	120.52
3	A	1043	LYS	CA-C-N	5.88	125.89	119.89
3	A	1043	LYS	C-N-CA	5.88	125.89	119.89
3	A	607	THR	N-CA-C	-5.80	106.20	113.28
3	A	664	ASP	CA-C-N	5.76	127.05	119.84
3	A	664	ASP	C-N-CA	5.76	127.05	119.84
3	A	426	TYR	CA-C-N	5.73	125.41	119.05
3	A	426	TYR	C-N-CA	5.73	125.41	119.05
3	A	572	THR	CB-CA-C	-5.72	99.96	111.17
2	D	5	DC	C5'-C4'-C3'	-5.71	106.33	114.90
3	A	672	ILE	CB-CA-C	-5.57	102.16	111.29
2	D	5	DC	P-O3'-C3'	-5.55	111.87	120.20
2	D	11	DC	O3'-P-O5'	-5.51	95.74	104.00
3	A	1109	LEU	N-CA-C	-5.43	95.79	111.00
3	A	924	ASP	N-CA-C	-5.41	107.23	112.97
3	A	588	ARG	N-CA-C	5.40	117.02	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	668	LYS	N-CA-CB	-5.34	108.08	114.17
3	A	589	GLU	N-CA-C	-5.26	105.57	112.72
3	A	576	ILE	N-CA-C	5.24	120.24	109.34
3	A	476	GLY	N-CA-C	-5.15	100.97	113.18
2	D	5	DC	C4'-C3'-O3'	5.13	117.70	110.00
3	A	738	GLU	N-CA-C	-5.09	105.81	112.23
3	A	569	THR	N-CA-C	5.08	119.69	112.93
3	A	718	GLU	N-CA-C	5.06	117.21	110.53
3	A	1122	TRP	N-CA-C	-5.02	106.25	112.38
3	A	714	ASN	N-CA-C	5.01	116.75	107.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	310	0	169	9	0
2	D	380	0	213	20	0
3	A	5929	0	5962	381	0
4	A	1	0	0	0	0
5	A	39	0	0	12	0
5	C	6	0	0	0	0
5	D	3	0	0	1	0
All	All	6668	0	6344	406	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (406) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:662:VAL:HG22	3:A:663:LEU:H	1.10	1.16
3:A:603:LYS:HD3	3:A:735:HIS:CD2	1.82	1.13
3:A:525:THR:HG21	3:A:535:LYS:HE3	1.18	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1001:ARG:O	3:A:1001:ARG:HD3	1.47	1.12
3:A:522:MET:HE1	3:A:624:LEU:HD21	1.33	1.11
3:A:713:LYS:HG3	3:A:727:TYR:CZ	1.86	1.09
3:A:423:ILE:CD1	3:A:501:ILE:HA	1.88	1.03
3:A:603:LYS:HE2	3:A:735:HIS:NE2	1.74	1.02
3:A:482:ARG:NH2	3:A:639:ASP:HA	1.77	0.99
3:A:507:ARG:O	3:A:508:LYS:HG3	1.63	0.97
3:A:603:LYS:HD3	3:A:735:HIS:HD2	1.14	0.96
3:A:664:ASP:OD2	3:A:667:LEU:HD23	1.66	0.96
3:A:525:THR:HG21	3:A:535:LYS:CE	1.96	0.96
3:A:581:MET:HB3	3:A:582:PRO:HD3	1.49	0.94
3:A:590:GLU:HB3	3:A:591:GLU:OE1	1.68	0.93
3:A:713:LYS:CG	3:A:727:TYR:CZ	2.53	0.91
3:A:525:THR:CG2	3:A:535:LYS:HE3	1.99	0.91
3:A:526:ASP:HB3	3:A:605:LEU:HG	1.51	0.90
3:A:522:MET:CE	3:A:624:LEU:HD21	2.02	0.90
3:A:590:GLU:HG2	3:A:591:GLU:CD	1.97	0.90
2:D:17:DC:C5	2:D:17:DC:N1	2.36	0.89
3:A:590:GLU:HG2	3:A:591:GLU:OE2	1.73	0.89
3:A:713:LYS:HG3	3:A:727:TYR:OH	1.70	0.89
3:A:423:ILE:HD13	3:A:501:ILE:HA	1.55	0.89
3:A:1001:ARG:HD3	3:A:1001:ARG:C	1.94	0.89
3:A:522:MET:HE3	3:A:557:LEU:CD1	2.03	0.88
3:A:603:LYS:CE	3:A:809:ASP:OD2	2.22	0.87
3:A:662:VAL:HG22	3:A:663:LEU:N	1.81	0.87
3:A:437:THR:HG22	3:A:438:LYS:N	1.90	0.87
3:A:879:ILE:HD11	3:A:885:ARG:HD2	1.57	0.86
3:A:664:ASP:OD2	3:A:667:LEU:CD2	2.22	0.86
3:A:628:HIS:CD2	3:A:631:GLN:OE1	2.28	0.85
3:A:662:VAL:CG2	3:A:663:LEU:H	1.88	0.85
3:A:526:ASP:CB	3:A:605:LEU:HG	2.07	0.85
3:A:437:THR:HG22	3:A:438:LYS:H	1.40	0.85
3:A:1030:ILE:HG22	3:A:1034:ILE:CD1	2.06	0.85
3:A:1120:ARG:O	3:A:1123:SER:HB3	1.76	0.85
3:A:581:MET:HB3	3:A:582:PRO:CD	2.06	0.85
3:A:1001:ARG:NH1	3:A:1005:TYR:CE2	2.44	0.84
3:A:477:LYS:NZ	3:A:533:HIS:ND1	2.26	0.84
3:A:603:LYS:CD	3:A:735:HIS:CD2	2.60	0.84
3:A:1044:PRO:HG2	3:A:1047:ALA:HB3	1.58	0.83
3:A:576:ILE:HG22	3:A:577:ALA:H	1.41	0.82
3:A:590:GLU:CG	3:A:591:GLU:CD	2.52	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:LEU:HD23	3:A:516:LEU:CD2	2.09	0.82
3:A:713:LYS:HG3	3:A:727:TYR:CE2	2.14	0.82
3:A:640:LEU:O	3:A:640:LEU:HD23	1.79	0.82
3:A:504:LEU:HD23	3:A:516:LEU:HD21	1.61	0.82
3:A:563:ILE:HD11	3:A:580:ASN:C	2.04	0.81
3:A:616:TYR:HA	3:A:623:HIS:CE1	2.15	0.81
3:A:599:GLN:NE2	3:A:601:TYR:CE1	2.49	0.81
3:A:713:LYS:HD2	3:A:727:TYR:CE1	2.15	0.81
3:A:495:ILE:O	3:A:499:LYS:HG3	1.81	0.80
3:A:477:LYS:NZ	3:A:533:HIS:HB3	1.97	0.80
3:A:576:ILE:HG22	3:A:577:ALA:N	1.96	0.80
3:A:1129:TYR:O	3:A:1133:LEU:HD13	1.83	0.78
3:A:872:TRP:NE1	3:A:902:GLU:OE2	2.16	0.78
3:A:653:TRP:CZ2	3:A:681:ILE:CG1	2.67	0.78
3:A:603:LYS:HE2	3:A:809:ASP:OD2	1.83	0.77
3:A:522:MET:HE3	3:A:557:LEU:HD12	1.64	0.77
3:A:888:GLY:HA3	3:A:902:GLU:O	1.85	0.77
3:A:507:ARG:O	3:A:508:LYS:CG	2.32	0.76
3:A:590:GLU:CB	3:A:591:GLU:OE1	2.33	0.76
3:A:1001:ARG:O	3:A:1001:ARG:CD	2.32	0.76
3:A:713:LYS:CD	3:A:727:TYR:CE2	2.69	0.76
3:A:681:ILE:O	3:A:685:LEU:HG	1.87	0.75
3:A:713:LYS:CD	3:A:727:TYR:CZ	2.69	0.75
3:A:603:LYS:CE	3:A:735:HIS:NE2	2.47	0.75
2:D:4:DG:H21	3:A:475:ARG:NH2	1.85	0.75
2:D:4:DG:H2''	2:D:5:DC:H5'	1.68	0.75
3:A:525:THR:CG2	5:A:33:HOH:O	2.34	0.75
3:A:590:GLU:HG2	3:A:591:GLU:OE1	1.86	0.75
3:A:872:TRP:CD1	3:A:902:GLU:OE2	2.40	0.75
3:A:757:ASN:OD1	3:A:843:PRO:CB	2.36	0.74
3:A:1001:ARG:HD2	3:A:1005:TYR:CE2	2.23	0.74
3:A:1167:GLN:HG3	5:A:36:HOH:O	1.88	0.74
3:A:590:GLU:CG	3:A:591:GLU:OE1	2.36	0.73
3:A:671:PRO:HG2	3:A:674:ASP:OD1	1.87	0.73
3:A:590:GLU:CG	3:A:591:GLU:OE2	2.35	0.73
3:A:585:GLU:O	3:A:589:GLU:OE1	2.06	0.73
3:A:939:ASP:HB3	3:A:1177:ARG:HG2	1.70	0.73
3:A:653:TRP:CZ2	3:A:681:ILE:HG13	2.23	0.73
3:A:849:ILE:HA	3:A:865:MET:HE1	1.71	0.73
3:A:526:ASP:HB2	3:A:605:LEU:H	1.52	0.72
3:A:586:LYS:O	3:A:590:GLU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:487:ASP:OD1	3:A:491:LYS:HE3	1.90	0.72
3:A:522:MET:HE3	3:A:557:LEU:HD13	1.70	0.72
3:A:713:LYS:HD2	3:A:727:TYR:CZ	2.22	0.72
3:A:762:LEU:HD12	3:A:786:GLU:HG3	1.69	0.72
3:A:573:LYS:O	3:A:574:ASN:C	2.28	0.72
3:A:603:LYS:CD	3:A:735:HIS:HD2	1.97	0.72
3:A:935:GLU:HG2	3:A:937:HIS:HE2	1.54	0.71
2:D:4:DG:C2'	2:D:5:DC:H5'	2.21	0.71
3:A:1030:ILE:CG2	3:A:1034:ILE:HD11	2.21	0.71
3:A:1061:ASN:HD21	3:A:1063:GLU:HG2	1.55	0.71
3:A:1030:ILE:HG22	3:A:1034:ILE:HD12	1.72	0.71
3:A:580:ASN:HB3	3:A:583:ASP:OD2	1.91	0.70
3:A:922:GLY:HA3	3:A:928:PRO:HD3	1.73	0.70
3:A:976:VAL:HG13	3:A:985:LYS:O	1.90	0.70
3:A:667:LEU:O	3:A:668:LYS:HB3	1.90	0.70
3:A:925:LYS:HB3	3:A:926:ILE:HD12	1.73	0.70
3:A:477:LYS:HZ2	3:A:533:HIS:CG	2.10	0.70
3:A:757:ASN:OD1	3:A:843:PRO:HB3	1.92	0.69
3:A:517:ARG:HA	5:A:8:HOH:O	1.92	0.69
3:A:640:LEU:O	3:A:640:LEU:CD2	2.41	0.68
3:A:643:SER:O	3:A:650:ARG:NH2	2.27	0.68
3:A:647:ALA:HA	3:A:650:ARG:NH1	2.09	0.68
3:A:532:SER:HA	3:A:535:LYS:HD2	1.75	0.68
3:A:674:ASP:O	3:A:678:LYS:HB2	1.93	0.67
3:A:1040:VAL:HG12	3:A:1048:ILE:HD11	1.76	0.67
3:A:653:TRP:CZ2	3:A:681:ILE:HG12	2.30	0.67
3:A:710:CYS:SG	3:A:715:LEU:HD22	2.34	0.67
3:A:437:THR:CG2	3:A:438:LYS:H	2.07	0.67
3:A:599:GLN:OE1	3:A:810:GLU:OE1	2.13	0.67
3:A:664:ASP:OD1	3:A:665:PRO:HD2	1.94	0.66
3:A:751:ASN:O	3:A:870:ARG:NH2	2.24	0.66
3:A:1001:ARG:HG3	3:A:1155:TRP:CZ2	2.30	0.66
3:A:560:ILE:HD11	3:A:625:LYS:HE2	1.76	0.66
3:A:976:VAL:HG22	3:A:986:LYS:HA	1.76	0.66
3:A:522:MET:HE1	3:A:624:LEU:CD2	2.20	0.66
3:A:492:ASN:O	3:A:496:GLN:HG2	1.96	0.66
3:A:651:LYS:HG2	3:A:837:TRP:CE2	2.31	0.65
3:A:652:GLU:OE1	3:A:655:ARG:HD2	1.96	0.65
3:A:756:ASN:O	3:A:870:ARG:NH1	2.29	0.65
3:A:482:ARG:NH2	3:A:639:ASP:CA	2.55	0.65
3:A:620:LEU:O	3:A:620:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1030:ILE:HG22	3:A:1034:ILE:HD11	1.77	0.65
3:A:474:LEU:HD21	3:A:498:ILE:HD11	1.79	0.65
3:A:1067:TYR:HE2	3:A:1069:GLY:O	1.80	0.65
3:A:668:LYS:O	3:A:668:LYS:HG3	1.97	0.64
3:A:1001:ARG:NH1	3:A:1005:TYR:CZ	2.65	0.64
3:A:449:GLU:OE2	5:A:31:HOH:O	2.14	0.64
3:A:713:LYS:HD2	3:A:727:TYR:CD1	2.32	0.64
3:A:852:ASN:CG	3:A:865:MET:HE3	2.23	0.64
3:A:1120:ARG:O	3:A:1123:SER:CB	2.45	0.64
3:A:1123:SER:HA	3:A:1128:ARG:HD2	1.80	0.63
3:A:423:ILE:HD11	3:A:501:ILE:HA	1.78	0.63
3:A:672:ILE:O	3:A:675:PHE:N	2.31	0.63
3:A:713:LYS:CG	3:A:727:TYR:CE2	2.79	0.63
3:A:772:THR:O	3:A:775:LYS:HE2	1.99	0.63
3:A:893:ILE:HD13	3:A:899:GLU:HB2	1.80	0.63
3:A:522:MET:CE	3:A:557:LEU:HD13	2.28	0.63
3:A:455:SER:O	3:A:458:VAL:HG12	1.99	0.63
3:A:507:ARG:C	3:A:508:LYS:HG3	2.24	0.62
3:A:757:ASN:OD1	3:A:843:PRO:HB2	1.98	0.62
3:A:1008:ARG:O	3:A:1012:MET:HG3	2.00	0.62
3:A:1137:GLN:HA	3:A:1140:GLU:OE1	2.00	0.62
3:A:482:ARG:HH22	3:A:638:ILE:C	2.08	0.61
3:A:630:LEU:CD1	3:A:672:ILE:CD1	2.78	0.61
3:A:467:ASP:HB3	3:A:468:TYR:CD2	2.36	0.61
3:A:477:LYS:HZ3	3:A:533:HIS:HB3	1.63	0.61
3:A:653:TRP:NE1	3:A:681:ILE:HD11	2.16	0.61
3:A:651:LYS:HE3	3:A:836:GLY:O	2.00	0.61
3:A:522:MET:CE	3:A:624:LEU:CD2	2.78	0.60
3:A:831:GLU:HG2	3:A:840:TYR:HD1	1.64	0.60
3:A:979:ASP:HB2	3:A:980:PRO:CD	2.30	0.60
3:A:1126:LYS:O	3:A:1130:GLN:HG2	2.01	0.60
3:A:576:ILE:CG2	3:A:577:ALA:H	2.11	0.60
3:A:502:MET:O	3:A:516:LEU:HB3	2.02	0.60
1:C:4:DA:H2''	1:C:5:DG:O4'	2.02	0.59
3:A:918:LEU:HD11	3:A:923:ASN:HB2	1.83	0.59
3:A:725:ALA:N	3:A:726:PRO:HD2	2.16	0.59
3:A:852:ASN:ND2	3:A:865:MET:HE3	2.18	0.59
3:A:526:ASP:CB	3:A:605:LEU:H	2.15	0.59
3:A:1029:PHE:CD2	3:A:1116:LEU:HD22	2.38	0.59
3:A:449:GLU:OE1	3:A:526:ASP:OD1	2.21	0.59
3:A:568:ILE:HG22	3:A:572:THR:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:935:GLU:HG2	3:A:937:HIS:NE2	2.17	0.59
3:A:661:THR:O	3:A:661:THR:HG22	2.03	0.58
3:A:935:GLU:O	3:A:936:GLN:HG3	2.03	0.58
3:A:433:ASN:HB2	3:A:467:ASP:HA	1.85	0.58
3:A:477:LYS:NZ	3:A:533:HIS:CB	2.67	0.58
3:A:1110:TYR:N	3:A:1110:TYR:CD2	2.70	0.58
3:A:504:LEU:HD23	3:A:516:LEU:HD22	1.85	0.57
3:A:664:ASP:OD2	3:A:667:LEU:HD21	2.04	0.57
1:C:12:DG:H2'	1:C:12:DG:O5'	2.03	0.57
3:A:664:ASP:CG	3:A:667:LEU:HD23	2.29	0.57
3:A:1110:TYR:N	3:A:1110:TYR:HD2	2.01	0.57
3:A:630:LEU:HD12	3:A:672:ILE:HD12	1.86	0.57
3:A:522:MET:HE2	3:A:624:LEU:HG	1.86	0.57
2:D:9:DG:OP1	3:A:650:ARG:NH1	2.37	0.57
3:A:609:LEU:HB2	3:A:612:GLU:HG3	1.87	0.57
3:A:526:ASP:HB3	3:A:605:LEU:CG	2.30	0.57
3:A:479:LEU:CD2	3:A:492:ASN:HD22	2.18	0.56
3:A:433:ASN:HD22	3:A:466:ARG:C	2.13	0.56
3:A:632:GLY:O	3:A:633:ASN:HB2	2.06	0.56
3:A:674:ASP:HB2	3:A:678:LYS:HG3	1.87	0.56
3:A:706:VAL:HA	3:A:728:VAL:HG11	1.88	0.56
3:A:872:TRP:CH2	3:A:886:MET:HG3	2.41	0.56
3:A:888:GLY:CA	3:A:902:GLU:O	2.52	0.56
3:A:762:LEU:HD12	3:A:786:GLU:CG	2.34	0.56
2:D:14:DC:H2''	2:D:15:DC:OP2	2.05	0.56
3:A:602:TYR:HA	3:A:607:THR:HG21	1.88	0.56
3:A:526:ASP:HB2	3:A:605:LEU:N	2.19	0.56
3:A:599:GLN:NE2	3:A:601:TYR:CZ	2.74	0.56
3:A:475:ARG:NH2	5:A:25:HOH:O	2.39	0.55
3:A:881:PRO:O	3:A:882:LEU:HB2	2.06	0.55
2:D:4:DG:H21	3:A:475:ARG:HH21	1.51	0.55
3:A:479:LEU:HD22	3:A:492:ASN:HD22	1.71	0.55
3:A:925:LYS:HB3	3:A:926:ILE:CD1	2.35	0.55
3:A:749:ALA:O	3:A:763:PRO:HG3	2.05	0.55
3:A:710:CYS:CB	3:A:715:LEU:HD22	2.37	0.55
3:A:429:LEU:HD12	3:A:471:CYS:O	2.06	0.55
3:A:1130:GLN:OE1	3:A:1130:GLN:HA	2.07	0.55
3:A:1024:SER:OG	3:A:1136:LYS:HE2	2.07	0.55
3:A:799:ASP:OD2	3:A:1001:ARG:NH2	2.31	0.54
3:A:1001:ARG:C	3:A:1001:ARG:CD	2.77	0.54
3:A:664:ASP:OD1	3:A:665:PRO:CD	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1030:ILE:CG2	3:A:1034:ILE:CD1	2.79	0.54
3:A:664:ASP:HB3	3:A:667:LEU:HG	1.88	0.54
3:A:947:LEU:HB2	3:A:952:MET:HG2	1.88	0.54
3:A:433:ASN:ND2	3:A:466:ARG:HB3	2.23	0.54
3:A:1065:LYS:NZ	3:A:1065:LYS:HB3	2.22	0.54
3:A:1061:ASN:ND2	3:A:1063:GLU:HG2	2.22	0.54
3:A:525:THR:OG1	3:A:531:GLY:CA	2.56	0.53
3:A:576:ILE:CG2	3:A:577:ALA:N	2.68	0.53
3:A:734:TYR:CE2	3:A:736:HIS:HB2	2.43	0.53
3:A:575:THR:O	3:A:575:THR:HG22	2.07	0.53
3:A:601:TYR:CB	3:A:603:LYS:NZ	2.72	0.53
3:A:725:ALA:O	3:A:741:LEU:CD2	2.56	0.52
2:D:18:DG:H2"	2:D:19:DG:OP2	2.09	0.52
3:A:588:ARG:NH2	3:A:810:GLU:CD	2.68	0.52
3:A:639:ASP:C	3:A:641:ALA:H	2.17	0.52
3:A:580:ASN:OD1	3:A:581:MET:N	2.40	0.52
3:A:479:LEU:CB	3:A:492:ASN:ND2	2.74	0.51
3:A:1016:LEU:HD22	3:A:1139:LYS:HD2	1.91	0.51
3:A:568:ILE:CG2	3:A:572:THR:HG23	2.40	0.51
2:D:16:DT:H2"	2:D:17:DC:OP2	2.10	0.51
3:A:601:TYR:HB2	3:A:603:LYS:HZ2	1.76	0.51
3:A:588:ARG:HA	3:A:592:SER:HB3	1.93	0.51
3:A:721:VAL:HG23	3:A:780:ALA:HB1	1.93	0.51
3:A:1049:ILE:CG2	3:A:1117:LEU:HD11	2.41	0.51
3:A:423:ILE:HG23	5:A:7:HOH:O	2.10	0.51
3:A:523:ILE:HD13	3:A:538:ILE:HD12	1.92	0.51
3:A:664:ASP:OD1	3:A:665:PRO:N	2.43	0.51
3:A:543:GLU:HB2	3:A:550:LEU:HD12	1.92	0.50
3:A:713:LYS:HD3	3:A:727:TYR:CE2	2.45	0.50
5:D:49:HOH:O	3:A:644:LYS:HA	2.11	0.50
3:A:437:THR:C	3:A:439:GLU:H	2.18	0.50
3:A:522:MET:SD	3:A:624:LEU:HD11	2.51	0.50
3:A:630:LEU:CD1	3:A:672:ILE:HD11	2.42	0.50
3:A:731:CYS:CB	5:A:18:HOH:O	2.58	0.50
3:A:1061:ASN:HD21	3:A:1063:GLU:CG	2.23	0.50
3:A:447:LEU:HG	3:A:521:LEU:HD11	1.92	0.50
3:A:681:ILE:O	3:A:681:ILE:HG22	2.11	0.50
3:A:857:MET:HE1	3:A:1156:ASN:OD1	2.12	0.50
3:A:477:LYS:NZ	3:A:533:HIS:CG	2.78	0.50
3:A:482:ARG:HH22	3:A:639:ASP:N	2.10	0.50
3:A:616:TYR:HA	3:A:623:HIS:HE1	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:731:CYS:HB2	5:A:18:HOH:O	2.12	0.49
3:A:979:ASP:HB2	3:A:980:PRO:HD2	1.94	0.49
3:A:1053:GLU:CD	3:A:1059:ARG:HH22	2.20	0.49
3:A:710:CYS:HB3	3:A:715:LEU:HD22	1.95	0.49
3:A:1156:ASN:O	3:A:1160:LYS:HG3	2.13	0.49
3:A:878:GLU:HB2	3:A:884:TYR:CE2	2.47	0.49
3:A:648:ASP:O	3:A:651:LYS:HB2	2.12	0.49
3:A:599:GLN:OE1	3:A:810:GLU:CD	2.56	0.49
3:A:1175:GLU:O	3:A:1175:GLU:HG2	2.08	0.49
3:A:482:ARG:NH2	3:A:638:ILE:C	2.72	0.48
3:A:668:LYS:O	3:A:668:LYS:CG	2.60	0.48
3:A:710:CYS:SG	3:A:715:LEU:CD2	3.01	0.48
3:A:725:ALA:HB3	3:A:726:PRO:HD3	1.94	0.48
3:A:729:SER:HB2	3:A:741:LEU:HD22	1.95	0.48
3:A:721:VAL:CG1	3:A:785:THR:HG23	2.43	0.48
2:D:17:DC:C2'	2:D:18:DG:C8	2.96	0.48
1:C:2:DC:H2'	1:C:3:DG:C8	2.48	0.48
3:A:713:LYS:CG	3:A:727:TYR:OH	2.52	0.48
3:A:578:PHE:CD1	3:A:584:TYR:HA	2.49	0.48
3:A:578:PHE:CD1	3:A:584:TYR:HB2	2.48	0.48
1:C:2:DC:H6	1:C:2:DC:O5'	1.96	0.48
3:A:479:LEU:HB3	3:A:492:ASN:ND2	2.29	0.48
3:A:601:TYR:CB	3:A:603:LYS:HZ1	2.26	0.48
3:A:713:LYS:CD	3:A:727:TYR:CD2	2.96	0.48
3:A:476:GLY:O	3:A:477:LYS:C	2.55	0.48
3:A:455:SER:C	3:A:458:VAL:HG12	2.39	0.48
3:A:603:LYS:HE3	3:A:809:ASP:OD2	2.10	0.48
3:A:923:ASN:HB3	3:A:926:ILE:H	1.79	0.48
2:D:5:DC:H2''	2:D:6:DA:H8	1.79	0.47
3:A:456:LEU:HB2	3:A:524:MET:HE1	1.96	0.47
3:A:1026:GLN:O	3:A:1029:PHE:HB3	2.13	0.47
3:A:603:LYS:CE	3:A:735:HIS:CD2	2.97	0.47
3:A:799:ASP:HB2	5:A:17:HOH:O	2.14	0.47
3:A:882:LEU:HD22	3:A:972:LEU:HB2	1.97	0.47
3:A:713:LYS:HD3	3:A:727:TYR:CD2	2.49	0.47
3:A:799:ASP:CG	3:A:1001:ARG:HH22	2.19	0.47
3:A:641:ALA:O	3:A:650:ARG:NE	2.48	0.47
3:A:805:TYR:CE2	3:A:815:PRO:HG3	2.49	0.47
3:A:497:ALA:O	3:A:501:ILE:HG12	2.15	0.47
3:A:522:MET:CE	3:A:624:LEU:HD11	2.45	0.47
3:A:522:MET:HE2	3:A:624:LEU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:588:ARG:C	3:A:590:GLU:H	2.23	0.47
3:A:725:ALA:O	3:A:741:LEU:HD23	2.13	0.47
3:A:817:TRP:HZ3	3:A:819:LEU:HD22	1.80	0.47
3:A:570:LYS:HA	3:A:571:PRO:HA	1.58	0.47
3:A:792:ARG:HB2	5:A:14:HOH:O	2.14	0.47
3:A:823:PRO:HD3	3:A:997:PHE:CD2	2.49	0.47
3:A:525:THR:CG2	3:A:535:LYS:CE	2.78	0.46
3:A:543:GLU:OE2	3:A:635:LYS:HG2	2.15	0.46
3:A:696:LEU:HD11	3:A:980:PRO:HG3	1.97	0.46
3:A:954:LYS:O	3:A:958:ILE:HG13	2.14	0.46
3:A:1001:ARG:HD2	3:A:1005:TYR:HE2	1.74	0.46
3:A:1144:GLU:O	3:A:1148:LYS:HG2	2.15	0.46
2:D:7:DT:H2''	2:D:8:DC:O4'	2.16	0.46
3:A:556:LEU:HG	3:A:627:PHE:CD1	2.50	0.46
3:A:581:MET:CB	3:A:582:PRO:CD	2.85	0.46
3:A:620:LEU:O	3:A:624:LEU:HB2	2.16	0.46
3:A:800:ASP:N	3:A:801:PRO:CD	2.79	0.46
3:A:856:LEU:HG	3:A:862:LEU:HD21	1.96	0.46
3:A:804:LYS:HD3	3:A:816:GLU:OE2	2.15	0.46
3:A:899:GLU:HG3	3:A:944:ILE:HG12	1.96	0.46
3:A:482:ARG:HH21	3:A:639:ASP:HA	1.73	0.46
3:A:849:ILE:HA	3:A:865:MET:CE	2.42	0.46
3:A:570:LYS:H	3:A:596:THR:HB	1.80	0.46
3:A:1027:VAL:HG22	3:A:1133:LEU:HD12	1.97	0.46
3:A:458:VAL:HG13	3:A:459:ALA:N	2.30	0.46
3:A:667:LEU:O	3:A:668:LYS:CB	2.60	0.46
3:A:1123:SER:HA	3:A:1128:ARG:CD	2.46	0.46
3:A:563:ILE:HD11	3:A:581:MET:N	2.32	0.45
3:A:1005:TYR:CZ	3:A:1155:TRP:HA	2.51	0.45
3:A:483:GLU:OE2	3:A:645:LYS:HD2	2.16	0.45
3:A:715:LEU:HB2	3:A:787:LEU:HG	1.99	0.45
3:A:601:TYR:HB2	3:A:603:LYS:NZ	2.31	0.45
3:A:662:VAL:CG2	3:A:663:LEU:N	2.53	0.45
2:D:17:DC:H2''	2:D:18:DG:C8	2.52	0.45
3:A:455:SER:O	3:A:458:VAL:CG1	2.64	0.45
3:A:444:THR:HA	3:A:520:HIS:O	2.17	0.45
3:A:1152:LYS:O	3:A:1156:ASN:HB2	2.16	0.45
3:A:713:LYS:HD2	3:A:727:TYR:CE2	2.46	0.45
1:C:4:DA:C2'	1:C:5:DG:C8	2.99	0.44
3:A:1001:ARG:HD2	3:A:1005:TYR:CD2	2.51	0.44
3:A:487:ASP:OD1	3:A:491:LYS:CE	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1027:VAL:CG2	3:A:1133:LEU:HD12	2.47	0.44
3:A:479:LEU:CB	3:A:492:ASN:HD22	2.31	0.44
3:A:548:GLY:O	3:A:551:ASP:HB2	2.17	0.44
3:A:656:GLN:O	3:A:657:TYR:C	2.60	0.44
2:D:18:DG:C6	2:D:19:DG:C6	3.06	0.44
3:A:568:ILE:O	3:A:573:LYS:HA	2.17	0.44
3:A:1005:TYR:CE2	3:A:1155:TRP:CG	3.06	0.44
3:A:445:LEU:O	3:A:521:LEU:HD12	2.18	0.43
3:A:522:MET:CE	3:A:624:LEU:CG	2.96	0.43
3:A:653:TRP:CE2	3:A:681:ILE:HG12	2.53	0.43
1:C:1:DC:H2''	1:C:2:DC:C5	2.53	0.43
3:A:725:ALA:HB3	3:A:726:PRO:CD	2.47	0.43
3:A:474:LEU:CD2	3:A:498:ILE:HD11	2.48	0.43
3:A:681:ILE:O	3:A:681:ILE:CG2	2.67	0.43
3:A:938:ASP:HB3	3:A:940:ASN:ND2	2.34	0.43
3:A:560:ILE:CD1	3:A:625:LYS:HE2	2.45	0.43
3:A:590:GLU:HG3	3:A:591:GLU:CD	2.39	0.43
2:D:3:DC:H2''	2:D:4:DG:H5'	2.01	0.43
3:A:480:ASN:OD1	3:A:540:ASN:ND2	2.51	0.43
2:D:10:DT:OP1	3:A:651:LYS:NZ	2.39	0.43
2:D:18:DG:H2'	2:D:18:DG:O5'	2.19	0.43
3:A:1171:GLN:NE2	5:A:36:HOH:O	2.33	0.43
2:D:17:DC:H2'	2:D:18:DG:C8	2.54	0.42
3:A:568:ILE:HG21	3:A:572:THR:HG23	2.01	0.42
3:A:938:ASP:O	3:A:939:ASP:OD1	2.36	0.42
3:A:482:ARG:HA	3:A:483:GLU:HA	1.62	0.42
3:A:585:GLU:O	3:A:588:ARG:HB3	2.20	0.42
3:A:926:ILE:HD12	3:A:926:ILE:N	2.34	0.42
3:A:550:LEU:HD23	3:A:550:LEU:HA	1.81	0.42
3:A:710:CYS:O	3:A:713:LYS:O	2.37	0.42
3:A:757:ASN:O	3:A:870:ARG:HD3	2.19	0.42
2:D:15:DC:H2''	2:D:16:DT:OP2	2.19	0.42
3:A:504:LEU:H	3:A:516:LEU:HD22	1.85	0.42
3:A:648:ASP:HA	3:A:651:LYS:HD2	2.02	0.42
3:A:826:LEU:HD23	3:A:826:LEU:HA	1.89	0.42
3:A:1155:TRP:HD1	3:A:1155:TRP:O	2.02	0.42
3:A:1018:TRP:CZ3	3:A:1065:LYS:HB2	2.54	0.41
3:A:1029:PHE:CG	3:A:1116:LEU:HD22	2.55	0.41
3:A:701:PRO:O	3:A:705:LYS:HG3	2.20	0.41
3:A:987:TYR:HE2	3:A:996:GLU:OE2	2.03	0.41
3:A:1028:LYS:O	3:A:1032:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:DG:O5'	1:C:12:DG:C2'	2.68	0.41
3:A:434:LYS:HD2	3:A:439:GLU:OE1	2.20	0.41
3:A:581:MET:O	3:A:584:TYR:N	2.53	0.41
3:A:634:ASP:HB3	3:A:672:ILE:HD12	2.01	0.41
3:A:954:LYS:HG2	3:A:958:ILE:HD11	2.01	0.41
3:A:591:GLU:O	3:A:594:LYS:HB2	2.21	0.41
3:A:482:ARG:NH2	3:A:639:ASP:N	2.68	0.41
3:A:550:LEU:HB2	3:A:630:LEU:HD22	2.03	0.41
3:A:674:ASP:HB2	3:A:678:LYS:CG	2.50	0.41
3:A:968:SER:HA	3:A:969:PRO:HD3	1.80	0.41
2:D:15:DC:H1'	2:D:16:DT:O5'	2.21	0.41
3:A:889:ARG:HE	3:A:902:GLU:HB2	1.85	0.41
3:A:1065:LYS:HA	3:A:1066:PRO:HD2	1.73	0.41
3:A:572:THR:C	3:A:573:LYS:CG	2.93	0.41
3:A:653:TRP:CE2	3:A:681:ILE:CG1	3.04	0.41
3:A:848:GLU:O	3:A:865:MET:HE2	2.21	0.41
3:A:1011:HIS:O	3:A:1015:ARG:HG2	2.21	0.41
3:A:433:ASN:HD21	3:A:466:ARG:HB3	1.85	0.41
3:A:495:ILE:HB	3:A:541:PHE:CE1	2.56	0.41
3:A:525:THR:HG23	5:A:33:HOH:O	2.13	0.41
3:A:713:LYS:HD2	3:A:727:TYR:CG	2.56	0.41
1:C:4:DA:H2''	1:C:5:DG:C8	2.56	0.40
3:A:437:THR:C	3:A:439:GLU:N	2.78	0.40
3:A:584:TYR:C	3:A:586:LYS:N	2.79	0.40
3:A:630:LEU:HD11	3:A:672:ILE:CD1	2.51	0.40
3:A:725:ALA:HB3	3:A:738:GLU:OE1	2.22	0.40
3:A:760:LEU:HA	3:A:791:THR:OG1	2.21	0.40
3:A:938:ASP:OD1	3:A:938:ASP:C	2.64	0.40
1:C:2:DC:N3	1:C:3:DG:C6	2.90	0.40
3:A:592:SER:HB2	3:A:597:TRP:CZ2	2.55	0.40
3:A:433:ASN:ND2	3:A:466:ARG:CB	2.85	0.40
3:A:667:LEU:HD22	3:A:667:LEU:HA	1.85	0.40
3:A:489:ILE:HG13	3:A:490:LEU:N	2.36	0.40
3:A:1121:ILE:C	3:A:1123:SER:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	717/759 (94%)	650 (91%)	64 (9%)	3 (0%)	30	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	504	LEU
3	A	813	VAL
3	A	673	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	640/674 (95%)	612 (96%)	28 (4%)	25	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	490	LEU
3	A	511	GLU
3	A	549	LEU
3	A	573	LYS
3	A	575	THR
3	A	595	PHE
3	A	600	LYS
3	A	620	LEU

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Mol	Chain	Res	Type
3	A	630	LEU
3	A	667	LEU
3	A	703	GLN
3	A	738	GLU
3	A	775	LYS
3	A	781	ARG
3	A	792	ARG
3	A	822	LEU
3	A	838	SER
3	A	906	ARG
3	A	930	ILE
3	A	1001	ARG
3	A	1006	GLN
3	A	1048	ILE
3	A	1065	LYS
3	A	1110	TYR
3	A	1126	LYS
3	A	1128	ARG
3	A	1167	GLN
3	A	1175	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	433	ASN
3	A	492	ASN
3	A	527	GLN
3	A	529	HIS
3	A	540	ASN
3	A	593	HIS
3	A	628	HIS
3	A	736	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	15/15 (100%)	0.50	0 100 100	36, 68, 113, 122	0
2	D	19/19 (100%)	0.57	1 (5%) 32 16	36, 54, 116, 117	0
3	A	721/759 (94%)	0.32	48 (6%) 24 12	18, 50, 106, 188	0
All	All	755/793 (95%)	0.33	49 (6%) 25 13	18, 51, 108, 188	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	640	LEU	5.1
3	A	665	PRO	4.4
3	A	1123	SER	4.2
3	A	674	ASP	4.1
3	A	572	THR	4.1
3	A	615	GLU	3.6
3	A	576	ILE	3.5
3	A	1121	ILE	3.5
3	A	547	LEU	3.3
3	A	482	ARG	3.2
3	A	1176	ALA	3.2
3	A	664	ASP	3.1
3	A	499	LYS	3.1
3	A	1177	ARG	3.0
3	A	666	THR	3.0
3	A	1122	TRP	2.9
3	A	668	LYS	2.8
3	A	680	LEU	2.8
3	A	607	THR	2.7
3	A	503	GLY	2.7
2	D	17	DC	2.6
3	A	571	PRO	2.6
3	A	669	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	1124	LEU	2.6
3	A	478	MET	2.5
3	A	603	LYS	2.5
3	A	644	LYS	2.5
3	A	1109	LEU	2.5
3	A	1034	ILE	2.4
3	A	567	SER	2.3
3	A	508	LYS	2.3
3	A	1129	TYR	2.3
3	A	667	LEU	2.3
3	A	757	ASN	2.3
3	A	1070	SER	2.3
3	A	580	ASN	2.3
3	A	789	LYS	2.2
3	A	599	GLN	2.2
3	A	507	ARG	2.2
3	A	575	THR	2.2
3	A	656	GLN	2.2
3	A	914	GLU	2.2
3	A	939	ASP	2.2
3	A	506	HIS	2.1
3	A	808	GLU	2.1
3	A	713	LYS	2.0
3	A	574	ASN	2.0
3	A	589	GLU	2.0
3	A	715	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	1	1/1	0.96	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.